

**REMARKS**

In the office action, the Examiner (1) rejected claims 5-16 and 19-21 under 35 U.S.C. § 102(a) as being anticipated by an article by Glendening et al. (“Glendening”), and (2) rejected claims 5, 11, 15 and 20 under 35 U.S.C. § 102(b) as being anticipated by an article by Graovac et al. (“Graovac”). Reconsideration and allowance of the application are requested.

**I. Glendening Rejection**

Independent claim 5 of the present application is directed to a computer-implemented method for use in deriving fixed bond information. The method features the steps of analyzing a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized structure representation describes a polycyclic ring system; identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure; evaluating at least a subset of the fixed bond representation candidates; selecting from among the plurality of fixed bond representation candidates based on the evaluation; producing fixed bond information based on the selection; and outputting the fixed bond information.

Glendening discloses a quantum-mechanical resonance theory. The reference does not disclose or suggest the steps of claim 5. In particular, Glendening does not disclose or suggest analyzing a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing. Glendening states on p. 602, under the heading “Generation of Resonance Structures” that “[g]iven wave function  $\psi$ , the NRT program constructs a list of one or more parent “reference” Lewis structures that describe the leading delocalization in the molecule.” Glendening, therefore, does not analyze a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing. Glendening, by contrast, only operates on a wave function.

In addition, Glendening does not disclose or suggest identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. The Examiner states that Glendening’s methodology relies on valence theory

in establishing resultant fixed bond structure on page 597, lines 34-39. Glendening, however, does not disclose how he enumerates resonance structures. The sentence cited by the Examiner only states that Glendening's structures are in "agreement" with elementary valence theory, not that valence theory is used in the methodology of deriving the resonance structures. Glendening, therefore, does not disclose identifying, *based on valence information*, a plurality of fixed bond representation candidates for at least a portion of the chemical structure.

Claim 5 is therefore patentable over Glendening. Claims 6-8, 11, 15, 16, 19 and 22 are dependent on claim 5 and are also allowable over Glendening.

Independent claim 9 is directed to a method for use in deriving fixed bond information. The method includes analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing; and identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Neither of these steps is disclosed or suggested by Glendening. Claim 9 is therefore patentable over Glendening.

Independent claim 10 includes the steps of analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing; and identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Neither of these steps is disclosed or suggested by Glendening. Claim 10 is therefore also allowable over Glendening.

Independent claim 12 includes the steps of analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing; and identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Neither of these steps is disclosed or suggested by Glendening. Claim 12 and its dependent claims 13 and 14 are therefore also allowable over Glendening.

Independent claim 20 is directed to a computer-implemented system for use in deriving fixed bond information. The system includes an analyzer analyzing a delocalized representation

of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized representation describes a polycyclic ring system; and an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. These elements are not disclosed or suggested by Glendening. Claim 20 is therefore patentable over Glendening.

Independent claim 21 is directed to computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to: analyze a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized representation describes a polycyclic ring system; and identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. The claimed software is neither disclosed nor suggested by Glendening. Claim 21 is therefore patentable over Glendening.

## II. Graovac Rejection

Graovac does not disclose or suggest the steps recited in independent claim 5. First, Graovac does not derive a fixed bond representation from a delocalized representation of a chemical structure. Graovac is only concerned with determining the relative contribution (i.e., the Kekulé index) of a particular (given) fixed bond representation with respect to the manifold of alternative valence bond depictions. Contrary to the Examiner's assertions, Figs. 1 and 2 of Graovac do not disclose a delocalized structure representation. Moreover, even if Figs. 1 and 2 can be said to disclose delocalized structures, there is nothing in the reference to indicate that they are converted to fixed bond structures.

In addition, Graovac does not disclose or suggest a computer-implemented method for use in deriving fixed bond information, including the step of outputting the fixed bond information. Graovac, by contrast, only discloses human-made intuitive determinations of structures without use of a computer. Table 1 of the reference, which the Examiner contends

discloses a resultant set of arranged polycyclic ring structures with fixed bond information, was conjured without using any computer-implemented algorithm. Independent claim 5 is therefore allowable over Graovac.

Claim 11 is dependent on claim 5 and further specifies “wherein the step of identifying is performed based on electronic state and valence distribution (ESVD), and further comprising: queuing at least a subset of the ESVDs by priority.” (Such priority queuing can be used, e.g., for quickly developing the most promising fixed-bond representations while bond assignment is incomplete.) The claimed step is neither disclosed, nor suggested by Graovac. Graovac only computes a property value (Kekule Index) for each structure, which is a sorting process, not priority queuing. There would be no need or use for queuing in Graovac’s process. Claim 11 is therefore patentable over Graovac.

Independent claim 20 is directed to a computer-implemented system for use in deriving fixed bond information. The system includes an analyzer analyzing a delocalized representation of a chemical structure, and an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. These elements are not disclosed or suggested by Graovac for reasons similar to those indicated above. Claim 20 is therefore allowable over the art of record.

New claims 22-27 have been added. These claims further describe identifying a plurality of fixed bond representation candidates. Claims 22-27 are neither disclosed, nor suggested by either the Glendening or Graovac references.

Claims 5-16 and 19-27 are pending in the present application. As the application is now believed to be in condition for allowance, issuance of a Notice of Allowance is respectfully requested.

The Commissioner is hereby authorized to charge any fee deficiency associated with this submission, or credit any overpayment to Deposit Account No. 08-0219.

Application Serial No. 09/506,717  
Amendment dated December 13, 2005  
Reply to Office Action dated June 13, 2005

In the event that an extension of time is required, or that may be required in addition to that requested in a petition for an extension of time, the Commissioner is requested to grant a petition for that extension of which is required to make this response timely, and is hereby authorized to charge any fee for such, to deposit account number 08-0219.

Respectfully submitted,



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Rajesh Vallabh  
Reg. No. 35,761

Wilmer Cutler Pickering Hale and Dorr LLP  
60 State Street  
Boston, MA 02109  
617-526-6505

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